Fluctuations due to the nonlocal character of collisions

K. Morawetz[1,2]
[1] *Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany and*
[2] *Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany*

It is shown that the collision integral describing the nonlocal character of collisions leads to the same mean-field fluctuations as proposed by Boltzmann-Langevin pictures. It is argued that this appropriate collision integral contains the fluctuation-dissipation theorems in equilibrium itself and therefore there is no need to assume additionally stochasticity. This leads to tremendous simplifications in numerical simulation schemes.

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The question how to describe sufficiently the fluctuations in dynamical systems of many interacting particles is as old as the discovery of the Brownian motion. Different schemes have been developed in different branches of physics. Mostly additional stochasticity is assumed to account for such fluctuations. The goal of this paper is to show how the correct fluctuations can be described by a realistic collision scenario within the deterministic kinetic theory without ad-hoc assumptions about stochasticity. Here we will briefly outline the attempts in nuclear physics having its counterparts in other fields, of course.

It has been noticed in the beginning of the 80th that the time-dependent mean-field description (TDHF) of nuclear collisions cannot describe the experimental fluctuations of observables Q like mass, charge and momenta of emitted particles [1] if the naive expectation

$$\Delta Q^2(t) = \mathrm{Tr}[Q^2\hat\rho_n(t)] - [TrQ\hat\rho_n(t)]^2 \qquad (1)$$

with the TDHF density matrix $\hat\rho_n$ is applied. This deficiency has been cured by a variational approach [2, 3, 4, 5, 6] which leads to the propagation of fluctuations from t_0

$$\Delta Q^2(t_1) = \lim_{\eta\to 0}\frac{1}{2\eta^2}\mathrm{Tr}[\hat\rho_n(t_0,0) - \hat\rho_n(t_0,\eta)]^2 \qquad (2)$$

where $\hat\rho_n(t,\eta)$ evolves with the TDHF equation but with the boundary condition $\hat\rho_n(t,\eta) = \exp(-i\eta Q)\hat\rho_n(t)\exp(i\eta Q)$. In this way the fluctuations are obtained by propagating back in time but they become explicitly dependent on the observables Q. It has been shown that the expression (2) leads besides the TDHF fluctuation (1) to an additional part which can be described by higher order diagrams in the interaction [4]. The application of this procedure leads to a significant enhancement of the fluctuations [1, 7, 8]. The fact that higher order diagrams are necessary to describe more appropriate fluctuations shows that the collisions are not described appropriately in usual Boltzmann (BUU) simulations.

Alternatively there has been developed the time dependent generator coordinator method (TDGCM) [9, 10] which expands the wave function Ψ in a set of TDHF wave functions ϕ_N

$$|\Psi(t)\rangle = \sum_N |\phi_N(t)\rangle f_N(t) \qquad (3)$$

where the coefficients f_N are determined from minimizing the action. The TDGCM wave function leads to optimal fluctuations if the TDHF basic set $\phi_N(0)$ is chosen such that the variable Q becomes a generator of the path at finite time t. This TDGCM schema is equivalent to the above described Balian-Veneroni variational approach [2] in the random phase approximation (RPA) limit. The advantage of the TDGCM schema is that it provides for optimal paths. However, both schemes are too limited for practical applications since one can handle only small sets of collective correlation channels.

This practical limitation has led to the development of stochastic TDHF [10] which approximates the time evolution of the N-particle density operator $\hat\rho$ at a small time steps t_i by the diagonal elements of the expansion in TDHF density operators $\hat\rho_n$

$$\hat\rho(t_i) = \sum_n W_n\hat\rho_n(t_i) + \sum_{nn'} W_n P_{n'n} t_i[\hat\rho_{n'}(t_i) - \hat\rho_n(t_i)]. \qquad (4)$$

The transition probability is given by the matrix element of TDHF Slater states at time t_i

$$P_{nn'} = \frac{2\pi}{\hbar}|\langle n|V|n'\rangle|^2\delta(E_n - E'_n) \qquad (5)$$

which leads to a Monte Carlo method of evolving an initial state into an ensemble of Slater states with the probability $W_m = 1 - \sum_{n'} P_{n'n}t_i$ for $m = n$ and $W_m = P_{mn}$ for $m \neq n$.

The usually used Boltzmann collision terms with the inclusion of Pauli-blocking (BUU) cannot account for these fluctuations since the collisions are treated as ideal, i.e. local in space and time. Therefore there has been proposed another method of including more realistic fluctuations in the Boltzmann equation for the one-particle distribution f by adding a stochastic term δI to the collision integral, called Boltzmann - Langevin picture [11, 12, 13, 14, 15, 16, 17]

$$\frac{df}{dt} = (1-f)W_{\rm in} - fW_{\rm out} + \delta I \qquad (6)$$

where schematically the scattering - out and -in probability of a phase space cell is $W_{\rm out/in}$. This Boltzmann-Langevin equation can be formally derived from the stochastic TDHF equation (4) if the one-particle reduced density is traced out. This equation has been applied for simulation of heavy-ion collisions quite frequently [18, 19, 20, 21, 22, 23, 24, 25]. In these treatments the Langevin term in (6) is mostly assumed to be Markovian

$$\langle \delta I \rangle = 0, \qquad \langle \delta I(t) \delta I(t') \rangle = 2D\delta(t-t') \tag{7}$$

which leads with (6) to the equation of motion for the variance $\sigma^2 = \langle f^2 \rangle - \langle f \rangle^2$

$$\frac{d\sigma^2}{dt} = -\frac{2}{\tau}\sigma^2 + 2D \tag{8}$$

with $1/\tau = W_{\rm out} + W_{\rm in}$. From the stochastic TDHF equation (4) the form (7) follows precisely neglecting fluctuations in the potential i.e. higher order diagrams [10]. Again this is a hint that the collisions have to be treated more appropriately. Before suggesting a way to describe fluctuations more realistically, let us discuss some principle problems of Boltzmann-Langevin approaches.

We have in principle no reason to see the time evolution of the density operator stochastically since the basic van-Neumann equation is deterministic and subsequent derived equations should be so as well. The ad-hoc assumption about stochasticity can mimic the numerical noise unavoidable in solving such equations and to a certain extent higher-order correlations. Theoretically it is a problem since the collision integral emerges itself from averaging about small scale fluctuations [26]. Therefore it is ambiguous to divide correlations into an averaged collision integral and a stochastic term miming higher-order correlations. This has been sometimes motivated by the need of the fluctuation-dissipation theorem associating the collision integral with dissipation. In contrast one should observe that the fluctuation-dissipation theorem emerges itself from appropriate collision integrals alone since they vanish in equilibrium. This can be seen best from ring summation approximation (RPA, GW, bubble...) leading to the Lenard-Balescu collision integral [27, 28]. The latter one vanishes exactly if the quantum fluctuation-dissipation theorem is fulfilled. In other words if the collision integral is derived appropriately it leads to an equilibrium with correct fluctuation-dissipation theorem and there is no need for additional stochastic terms.

Introducing fluctuations the determination of f and the stochastic process δI remains phenomenological in the sense that they account partially for such an appropriate collision integral. This is a practical need if the appropriate collision integral is not solvable and one is restricted to Born (Boltzmann) approximation. Here in this letter we will show that the same mean fluctuations are generated from the deterministic but more realistic nonlocal extension of the Boltzmann collision integral [29, 30, 31, 32]. The advantage is that besides the microscopic foundation the latter one has already established a practical and fast numerical method.

Let us return to the Boltzmann-Langevin equation. The fluctuation term derived from stochastic TDHF leads to the educated guess [20]

$$2D = (1 - \langle f \rangle) W_{\rm in} + \langle f \rangle W_{\rm out} \tag{9}$$

which has suggested an interesting procedure to include fluctuations dynamically in BUU codes. From (8) one sees that the choice (9) reproduce the equilibrium variance $\sigma^2 = f_0(1-f_0)$ and that the deviation between the actual variance and the statistical value $\delta\sigma^2 = \sigma^2 - \langle f \rangle(1 - \langle f \rangle)$ obeys

$$\frac{d\delta\sigma^2}{dt} = -\frac{2}{\tau}\delta\sigma^2. \tag{10}$$

Since $\delta\sigma^2 = 0$ is a solution of (10), the averaged value $\langle f \rangle$ can be parametrized as local equilibrium value such that at a given phase-space cell and time a small propagation will not deviate the variance from this result [20]. Numerically the authors in [20] used instead of the variance in distribution the density projection

$$\sigma_n^2(r,t) = \frac{4}{V}\int \frac{dp}{\hbar^3} \langle f \rangle (1 - \langle f \rangle) \tag{11}$$

which has been realized in each phase-space point of collisions.

Besides the practical success of such descriptions in numerical solutions it remains the more principle question of the validity of the ad-hoc stochastic assumption. As we have pointed out this assumption partially cures the ideal collision scenario of space and time point-like particles. We will follow now the other point of view and claim that if the collisions are described more realistically by nonlocal events then the fluctuations should be correctly induced by itself.

The nonlocal extension of the Boltzmann equation has been given in [29, 30] and the finite duration and dynamical size of nucleons are calculated in [31]. The implementation in BUU codes has allowed to describe experimentally noticeable effects [32, 33, 34]. The prediction of a change in the reaction mechanisms [35] has been nicely confirmed by proper scaling of experimental data [36]. The correlations by the nonlocal character of collisions are capable to describe long range order as typical for phase transitions [33].

These nonlocal extensions are more realistic than the Boltzmann equation since they lead to the inclusion of two-particle correlations while in the Boltzmann equation these correlations are absent. We will show now that this more realistic description of the individual collision event induces also more realistic fluctuations which should be compared to the above described treatments. Especially

we will find that the nonlocal corrections lead to induced mean-field fluctuations of the form (11).

The nonlocal quasiparticle kinetic equation for the distribution function of particle a, $f_1 \equiv f_a(k,r,t)$, derived within the non-equilibrium Green's function technique [29, 30] has the form of a Boltzmann equation with the quasiparticle energy $\varepsilon_1 = \varepsilon(k,r,t)$

$$\frac{\partial f_1}{\partial t} + \frac{\partial \varepsilon_1}{\partial k}\frac{\partial f_1}{\partial r} - \frac{\partial \varepsilon_1}{\partial r}\frac{\partial f_1}{\partial k} = s\sum_b \int \frac{dpdq}{(2\pi)^5\hbar^7}\mathcal{P}_\pm \times\Big[\big(1-f_1\big)\big(1-f_2^-\big)f_3^-f_4^- - f_1 f_2^\pm\big(1-f_3^\pm\big)\big(1-f_4^\pm\big)\Big] \quad (12)$$

and the spin-isospin etc degeneracy s. The superscripts $\pm$ denote the signs of non-local corrections: $f_2^\pm \equiv f_b(p, r\pm\Delta_2, t)$, $f_3^\pm \equiv f_a(k-q\pm\Delta_K, r\pm\Delta_3, t\pm\Delta_t)$, and $f_4^\pm \equiv f_b(p+q\pm\Delta_K, r\pm\Delta_4, t\pm\Delta_t)$. For the out-scattering part of (12) both signs can be given equivalently [37]. The scattering measure is given by the modulus of the scattering T-matrix $\mathcal{P}_\pm = |\mathcal{T}_\pm^R|^2\delta(\varepsilon_1+\varepsilon_2-\varepsilon_3-\varepsilon_4\pm 2\Delta_E)$. All corrections, the Δ's, describing the non-local and non-instant collision are given by derivatives of the scattering phase shift $\phi = \mathrm{Im}\,\ln\mathcal{T}^R(\Omega,k,p,q,t,r)$

$$\begin{aligned}
\Delta_t &= \frac{\partial\phi}{\partial\Omega}\Big|_{\varepsilon_1+\varepsilon_2} & \Delta_2 &= \Big(\frac{\partial\phi}{\partial p} - \frac{\partial\phi}{\partial q} - \frac{\partial\phi}{\partial k}\Big)_{\varepsilon_1+\varepsilon_2}\\
\Delta_E &= -\frac{1}{2}\frac{\partial\phi}{\partial t}\Big|_{\varepsilon_1+\varepsilon_2} & \Delta_3 &= -\frac{\partial\phi}{\partial k}\Big|_{\varepsilon_1+\varepsilon_2}\\
\Delta_K &= \frac{1}{2}\frac{\partial\phi}{\partial r}\Big|_{\varepsilon_1+\varepsilon_2} & \Delta_4 &= -\Big(\frac{\partial\phi}{\partial k} + \frac{\partial\phi}{\partial q}\Big)_{\varepsilon_1+\varepsilon_2}.
\end{aligned} \quad (13)$$

The nonlocal kinetic equation (12) covers all quantum virial corrections on the binary level and conserves density, momentum and energy including the corresponding two-particle correlated parts [30]. It requires no more computational power than solving the Boltzmann equation [32, 34].

We will now derive the fluctuation contribution to the mean-field from this collision integral. Therefore we use the fact that the mean-field can be considered as zero-angle collisions, a collision which does not change momenta of particles but changes its phase. Summing up all these changes in phase gives just the mean-field potential due to the surrounding media. When deriving collision integrals one tries to share correlations in such a way that all mean-field like contributions are collected in the quasiparticle energies on the left side and all true collisions with finite transferred momenta are on the right side. In addition we will observe now that due to the nonlocal character of the collision there is a finite zero transfer momenta channel hidden in the nonlocal collision integral which can be rewritten into the drift side of the kinetic equation and which gives exactly the fluctuations (11).

To show this we rewrite the energy-conserving δ-function in (12) as

$$\begin{aligned}
&\delta\left(\frac{k^2}{2m_a} + \frac{p^2}{2m_b} - \frac{(k-q)^2}{2m_a} - \frac{(p+q)^2}{2m_b}\right)\\
&= \delta\left(|q|(\frac{k}{m_a} - \frac{p}{m_b})\cdot\frac{q}{|q|} - \frac{q^2}{2}(\frac{1}{m_a}+\frac{1}{m_b})\right)\\
&= \frac{\delta(|q|)}{\left(\frac{k}{m_a}-\frac{p}{m_b}\right)\cdot\frac{q}{|q|}} + \delta(q\neq 0)
\end{aligned} \quad (14)$$

where the channel $q \neq 0$ represents the usually collision integral of (12). The $q = 0$ channel leads now to an additional part absent in usual local kinetic equations like the Boltzmann equation. To convince the reader about this novel observation let us rewrite the Pauli-blocking factors of (12) for the $q = 0$ channel according to (14)

$$\begin{aligned}
&\Big[\big(1-f_1\big)\big(1-f_2^-\big)f_3^-f_4^- - f_1 f_2^\pm\big(1-f_3^\pm\big)\big(1-f_4^\pm\big)\Big]_{q=0}\\
&= f_2^-(1-f_2^-)\Big[f_1^- - f_1\Big].
\end{aligned} \quad (15)$$

We see that in the case of local kinetic equations without delays this specific channel disappears since $f_1^- = f_1$. Therefore in contrast to the usual local kinetic equations the nonlocal equation possesses a finite zero-angle channel in the collision integral which is of mean-field type since no energy or momenta is exchanged. The fact that retardation leads to an additional correction to the Bogoliubov–Hartree-Fock mean-field has been observed first within linear response in [38].

From (12) we obtain now

$$\frac{\partial f_1}{\partial t} + \frac{\partial \varepsilon_1}{\partial k}\frac{\partial f_1}{\partial r} - \frac{\partial \varepsilon_1}{\partial r}\frac{\partial f_1}{\partial k} = \frac{\langle f_1^- - f_1\rangle}{\tilde\tau} + s\int_{q\neq 0}\frac{dpdq}{(2\pi)^5\hbar^7}\mathcal{P}_\pm \times\Big[\big(1-f_1\big)\big(1-f_2^-\big)f_3^-f_4^- - f_1 f_2^\pm\big(1-f_3^\pm\big)\big(1-f_4^\pm\big)\Big] \quad (16)$$

where

$$\frac{1}{\tilde\tau} = \Big\langle \frac{2\pi s}{\hbar}\int\frac{dpdq}{(2\pi\hbar)^6}|\mathcal{T}^r|^2\delta\Big(\frac{k\cdot q}{m_a} - \frac{p\cdot q}{m_b}\Big) f_p(1-f_p)\Big\rangle. \quad (17)$$

Here we use the approximation of thermal averaged delays, $\langle ...\rangle$, which allows us to pull out the f_1^- term which contains the p-dependent shift under the integration of the $1/\tilde\tau$ term. This serves here for legibility and can be rendered exactly if one keeps the corresponding shift terms under the (p,q) integral of (17).

The resulting equation (16) is a delay-differential equation and has lead already to an interesting interplay between stochastic bifurcations and relaxation due to inertia [39]. We see from (16) and (17) that terms $1/\tilde\tau \propto \sigma^2$ of (11) appears. In order to see that this additional term represents mean-field fluctuations let us expand

$$\langle f_1 - f_1^-\rangle = \langle \Delta_t\frac{\partial f}{\partial t} + \Delta_3\frac{\partial f}{\partial r} + \Delta_K\frac{\partial f}{\partial k}\rangle \approx \tilde\Delta_3\frac{\partial f}{\partial r} + \tilde\Delta_K\frac{\partial f}{\partial k} \quad (18)$$

where in the last step we have replace the time derivative of f by the free drift motion $\frac{\partial f_1}{\partial t} \approx -\frac{\partial \varepsilon_1}{\partial k}\frac{\partial f_1}{\partial r} + \frac{\partial \varepsilon_1}{\partial r}\frac{\partial f_1}{\partial k}$ leading to the on-shell shifts

$$\begin{aligned} \tilde{\Delta}_3 &= \langle \Delta_3 - \Delta_t \frac{\partial \varepsilon_k}{\partial k} \rangle = -\langle \frac{\partial \phi^{on}}{\partial k} \rangle \\ \tilde{\Delta}_K &= \langle \Delta_K + \Delta_t \frac{\partial \varepsilon_k}{\partial r} \rangle = \langle \frac{\partial \phi^{on}}{\partial r} \rangle. \end{aligned} \tag{19}$$

Now we can shift (18) from the right to the left (drift) side of (16) to obtain finally

$$\begin{aligned} &\frac{\partial f_1}{\partial t} + \left(\frac{\partial \varepsilon_1}{\partial k} + \frac{\tilde{\Delta}_3}{\tilde{\tau}} \right) \frac{\partial f_1}{\partial r} - \left(\frac{\partial \varepsilon_1}{\partial r} - \frac{\tilde{\Delta}_K}{\tilde{\tau}} \right) \frac{\partial f_1}{\partial k} \\ &= s \sum_b \int_{q \neq 0} \frac{dpdq}{(2\pi)^5} \mathcal{P}_{\pm} \\ &\times \Big[\big(1-f_1\big)\big(1-f_2^-\big) f_3^- f_4^- - f_1 f_2^{\pm} \big(1-f_3^{\pm}\big)\big(1-f_4^{\pm}\big) \Big]. \end{aligned} \tag{20}$$

We see that an explicit fluctuating term $\sim 1/\tilde{\tau} \sim \sigma_n^2(r,t)$ emerges to the mean field which has the form of (11).

Therefore we conclude that the variance of fluctuations from the Langevin–Boltzmann equation can be reproduced in a deterministic way from the nonlocal extension of the Boltzmann equation. The stochastic treatment in numerical realizations can be considered therefore as a numerical trick to reproduce the correct deterministic fluctuations. The nonlocal collision scheme instead provides a first principle theory of such fluctuations. It gives probably the same practical results but with much less numerical effort since the collision scenario of the usual BUU code is modified only slightly with no additional computational time required [32, 34]. Therefore we have demonstrated that the ad-hoc assumption about Langevin sources to the Boltzmann equation is unnecessary if the collisions are treated non-locally.

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